Elementary Excitations of Quantum Critical 2+1 D Antiferromagnets

Zaira Nazario[†] and David I. Santiago^{†,*}

† Department of Physics, Stanford University, Stanford, California 94305

* Gravity Probe B Relativity Mission, Stanford, California 94305

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It has been proposed that there are degrees of freedom intrinsic to quantum critical points that can contribute to quantum critical physics. We point out that this conclusion is quite general below the upper critical dimension. We show that in 2+1 D antiferromagnets skyrmion excitations are stable at criticality and identify them as the critical excitations. We found exact solutions composed of skyrmion and antiskyrmion superpositions, which we call topolons. We include the topolons in the partition function and renormalize by integrating out small size topolons and short wavelength spin waves. We obtain correlation length exponent $\nu = 0.9297$ and anomalous dimension $\eta = 0.3381$.

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Quantum phase transitions have been a subject of theoretical and experimental exploration since the pioneering work of John Hertz[1]. Since then, quantum critical behavior has been understood and studied as arising from quantum fluctuations of the order parameter[1, 2]. In this traditional approach the quantum transition is studied via the Wilson renormalization group in which fluctuations of the order parameter are taken properly into account. It is said that quantum phase transitions follow the Landau-Ginzburg-Wilson paradigm (LGW).

It has recently been suggested that quantum critical points will have properties that cannot be obtained from LGW order parameter fluctuations alone[3, 4]. In particular, it was suggested that quantum critical points will have low energy elementary excitations intrinsic to the critical point whose fluctuations will contribute and modify the critical properties. It was postulated that these excitations will be fractionalized[3, 4].

That some quantum critical points have elementary excitations different from those of each of the phases it separates can be inferred quite generally. We concentrate in relativistic quantum critical points, but we emphasize that these physics can take place in other systems. For such a system, which we take to be an antiferromagnet, we are interested in the Nèel magnetization Green's function, or staggered magnetic susceptibility.

In the ordered phase the transverse Green function or susceptibility corresponds to spin wave propagation and it has a nonanalyticity in the form of a pole corresponding to such propagation:

$$\langle \vec{n}(-\omega, -\vec{k}) \cdot \vec{n}(\omega, \vec{k}) \rangle = \frac{Z(\omega, \vec{k})}{c^2 k^2 - \omega^2} + G_{\text{incoh}}(\omega, \vec{k}).$$

Here $Z(\omega, \vec{k})$ is between 0 and 1, and the incoherent background $G_{\rm incoh}$ vanishes at long wavelengths and small frequencies. The fact that the Green's function has a pole means that transverse Goldstone spin waves are low energy eigenstates of the antiferromagnet. At criticality, the system has no Nèel order and thus Goldstones cannot be elementary excitations of the system.

In the disordered phase the Green function or susceptibility corresponds to spin wave propagation with all three polarizations and it has a pole nonanalyticity corresponding to such propagation:

$$\langle \vec{n}(-\omega, -\vec{k}) \cdot \vec{n}(\omega, \vec{k}) \rangle = \frac{A(\omega, \vec{k})}{c^2 k^2 + \Delta^2 - \omega^2} + G_{\rm incoh}(\omega, \vec{k}) \,.$$

Here $A(\omega, \vec{k})$ is between 0 and 1, and the incoherent background $G_{\rm incoh}$ vanishes at long wavelengths and small frequencies, Δ is the gap to excitations in the disordered phase. That this Green's function has a pole means that triplet or triplon spin waves are low energy eigenstates of the disordered antiferromagnet. For 2+1 D antiferromagnets, and in general for antiferromagnets below the upper critical dimension, the quasiparticle pole residue A vanishes as the system is tuned to the quantum critical point[5]. At criticality, triplon excitations have no spectral weight and thus triplons cannot be elementary excitations of the system.

On the other hand right at criticality the response function below the upper critical dimension (below which $\eta \neq 0$, while above $\eta = 0$) has nonanalyticities that are worse than poles

$$\langle \vec{n}(-\omega, -\vec{k}) \cdot \vec{n}(\omega, \vec{k}) \rangle = A' \left(\frac{1}{c^2 k^2 - \omega^2} \right)^{1 - \eta/2}$$
 (1)

as obtained from the renormalization group studies of the nonlinear sigma model[5, 6]. Below the upper critical dimension η is a nonintegral universal number for each dimensionality. This critical susceptibility has no pole structure, but has a branch cut. It sharply diverges at $\omega=ck$ and is purely imaginary for $\omega>ck$. Branch cuts in quantum many-body or field theory represent immediate decay of the quantity whose Green function is being evaluated. Hence the elementary excitations or eigenstates of the noncritical quantum mechanical phases break up as soon as they are produced when the system is tuned to criticality: they do not have integrity. The complete lack of pole structure and the branch cut singularity below the upper critical dimension mean that the

elementary excitations of the quantum mechanical phases away from criticality, the spin waves, cannot even be approximate eigenstates at criticality as they are absolutely unstable.

The quantum critical point is a unique quantum mechanical phase of matter, which under any small perturbation becomes one of the phases it separates. It is a repulsive fixed point of the renormalization group. As far as the transition from one quantum mechanical phase to the other is continuous, and both phases have different physical properties, the critical point will have its unique physical properties different from the phases it separates. The properties of the critical point follow from the critical Hamiltonian $H(g_c)$ (g_c is the critical coupling constant), which will have a unique ground state and a collection of low energy eigenstates which are its elementary excitations. These low energy eigenstates are different from those of each of the phases as long as we are below the upper critical dimension. As a matter of principle, all quantum critical points below the upper critical dimension will have their intrinsic elementary excitations.

We have seen that below the upper critical dimension, the excitations of the stable quantum phases of the system become absolutely unstable and decay when the system is tuned to criticality. The question comes to mind immediately: what could they be decaying into? When one tries to create an elementary excitation of one of the phases, it will decay immediately into the elementary excitations of the critical point. The critical excitations will be bound states of the excitations of the stable phases the critical point separates. These bound states could be fractionalized as conjectured by Laughlin[3] and Senthil, et. al.[4], but they need not be in all cases. These critical degrees of freedom are responsible for corrections to the LGW phase transition canon[4]. The intrinsic quantum critical excitations contribute to the thermodynamical and/or physical properties of the quantum critical system.

Now we turn to a specific model in order to identify what the critical excitations are. We concentrate on 2 + 1 dimensional short-range Heisenberg antiferromagnets in a bipartite lattice. These are described by the O(3) nonlinear sigma model augmented by Berry phases [7, 8]

$$\mathcal{Z} = \int \mathcal{D}\vec{n}\delta(\vec{n}^2 - 1)e^{-\mathcal{S}_E}$$

$$\mathcal{S}_E = iS_B + \int_0^\beta d\tau \int d^2\vec{x} \frac{\rho_s}{2} \left[(\partial_{\vec{x}}\vec{n})^2 + \frac{(\partial_\tau \vec{n})^2}{c^2} \right] . \tag{2}$$

where $\rho_s \equiv JS^2$ is the spin stiffness, and the spin-wave velocity $c = 2\sqrt{2}JSa$ with a the lattice constant and J the microscopic spin exchange. The Berry phase terms represent the sums of the areas swept by the vectors $\vec{n}_i(\tau)$ on the surface of a unit sphere as they evolve in Euclidean time[7]. They were shown to be zero[7, 9] in the Nèel phase and the critical point, but relevant in the disor-

dered phase[10]. We drop the Berry phase terms as we will study the critical properties of 2+1 D antiferromagnets as approached from the Nèel phase.

The O(3) nonlinear sigma model action (2) has a classical "ground state" or lowest energy state with Nèel order corresponding to a constant magnetization. The equations of motion that follow from the action have approximate time dependent solutions, corresponding to Goldstone spin wave excitations. The equations of motion, in 2+1 D only, also have exact static solitonic solutions of finite energy[11]

$$E = \frac{\rho_s}{2} \int d^2 \vec{x} (\partial_i \vec{n})^2 = 4\pi \rho_s . \tag{3}$$

These solitons are called skyrmions[12].

Skyrmions are of a topological nature as they are characterized by the integer winding number

$$q = \frac{1}{8\pi} \int d^2x \epsilon^{ij} \vec{n} \cdot (\partial_i \vec{n} \times \partial_j \vec{n}) . \tag{4}$$

These configurations consist in the order parameter rotating an integer number of times as one moves from infinity toward a fixed but arbitrary position in the plane. Since two dimensional space can be thought of as an infinite 2 dimensional sphere where the magnetic moments live, the excitations fall in homotopy classes of a 2D sphere into a 2D sphere: $S^2 \to S^2[11]$. Skyrmions rotate at finite length scales but relax into the Néel state far away: $\lim_{|\vec{x}| \to \infty} \vec{n} = (0,0,-1)$. They have a directionality given by the direction of the Nèel order they relax to at infinity. The skyrmion number is a conserved quantum number as it is the zeroth component of the current $J^\mu = (1/8\pi)\epsilon^{\mu\nu\sigma}\vec{n}\cdot\partial_\nu\vec{n}\times\partial_\sigma\vec{n}$ which can easily be checked to be conserved $\partial_\mu J^\mu = 0$.

In order to study skyrmion properties more conveniently, we use a very useful way of describing the O(3) nonlinear sigma model, which is through the stereographic projection[11, 13]:

$$n^{1} + in^{2} = \frac{2w}{|w|^{2} + 1}, n^{3} = \frac{1 - |w|^{2}}{1 + |w|^{2}}, w = \frac{n^{1} + in^{2}}{1 + n^{3}}.$$
 (5)

In terms of w the nonlinear σ -model action is

$$S_E[w] = \frac{2\Lambda}{g_{\Lambda}} \int d\tau d^2x \frac{\partial^{\mu}w \partial_{\mu}w^*}{(1+|w|^2)^2} =$$

$$\frac{2\Lambda}{g_{\Lambda}} \int d\tau d^2x \frac{\partial_0 w \partial_0 w^* - 2\partial_z w \partial_{z^*} w^* - 2\partial_{z^*} w \partial_z w^*}{(1 + |w|^2)^2} , (6)$$

where z = x + iy and $z^* = x - iy$ is its conjugate, and $\Lambda/g_{\Lambda} = \rho_s$. g_{Λ} is the microscopic Goldstone coupling constant defined at the microscopic cutoff scale $\Lambda[5, 6]$. The classical equations of motion which follow by stationarity of the classical action are

$$\partial_0^2 w - 4\partial_z \partial_{z^*} w = \frac{2w^*}{1 + |w|^2} \left[(\partial_0 w)^2 - 4\partial_z w \partial_{z^*} w \right] = 0$$

When the system Nèel orders, \vec{n} , or equivalently w, will acquire an expectation value: $\langle n^a \rangle = \delta^{3a}$, $\langle w \rangle = 0$.

As mentioned above, besides Goldstones, there are static skyrmion configurations[11, 13]: $w = \prod_{i=1}^{q} \lambda/(z - a_i)$ whose topological invariant (4) in terms of the stereographic variable, w, is

$$q = \frac{1}{\pi} \int d^2x \frac{\partial_z w \partial_{z^*} w^* - \partial_{z^*} w \partial_z w^*}{(1 + |w|^2)^2} \,. \tag{7}$$

This configuration can easily be checked to have charge q and energy $4\pi q\Lambda/g_{\Lambda}$. λ^q is the arbitrary size and phase of the configuration and a_i are the positions of the skyrmions that constitute the multiskyrmion configuration. Similarly, the multiantiskyrmion configuration can be shown to be $w=\prod_{i=1}^q \lambda^*/(z^*-a_i^*)$ with charge -q and energy $4\pi q\Lambda/g_{\Lambda}$.

We now investigate whether skyrmions and antiskyrmion configurations are relevant at the quantum critical point. As mentioned above, their classical energy is $4\pi\Lambda/g_{\Lambda}$, which is independent of the size of the skyrmion λ . On the other hand, in real physical systems there are quantum and thermal fluctuations. These renormalize the effective coupling constant of the nonlinear sigma model and makes it scale dependent. To one loop order the renormalized coupling constant is

$$g_{\mu} = \frac{\mu}{\Lambda} \frac{g_{\Lambda}}{1 - (g_{\Lambda}/2\pi^2) (1 - \mu/\Lambda)}.$$
 (8)

Since the skyrmion has an effective size λ , spin waves of wavelength smaller than λ renormalize the energy of the skyrmion via the coupling constant renormalization leading to an energy and Euclidean action $S_E = \beta E$, which are now scale dependent through the scale dependence of the coupling constant at scale $\mu = 1/\lambda$. If the system is at temperature $T = 1/\beta$, this temperature sets the size of the skyrmion to be the thermal wavelength $\lambda = \beta$. The skyrmion Euclidean action is then

$$S_E = \frac{8\pi\beta}{\beta g_{1/\beta}} = \frac{8\pi\beta\Lambda}{g_\Lambda} \left[1 - \frac{g_\Lambda}{2\pi^2} \left(1 - \frac{1}{\beta\Lambda} \right) \right]$$
(9)

Having obtained the Euclidean action for skyrmions (9), we now study its low temperature limit in the Nèel ordered phase and at the quantum critical point. According to the one loop renormalized coupling constant (8), the quantum critical point occurs when the renormalized spin stiffness $(\rho_s(\mu) \propto \mu/g_\mu)$ vanishes at long wavelengths $(\mu \to 0)$: $g_{\Lambda} = g_c = 2\pi^2$. Since the skyrmion gap is $4\pi\mu/g_{\mu}$, the critical point corresponds to skyrmion gap collapse. When in the Nèel ordered phase, $g_{\Lambda} < g_c$, the skyrmion Euclidean action (9) is infinite. Therefore, the probability for skyrmion contributions is suppressed exponentially at low temperatures, vanishing at zero temperature. Skyrmions are gapped and hence irrelevant to low temperature physics in the Nèel ordered phase.

At the quantum critical point $g_{\Lambda} = g_c = 2\pi^2$, the skyrmion Euclidean action is

$$S_E = \frac{4}{\pi} \,. \tag{10}$$

This action is finite and constant at all temperatures and in particular, it will have a nonzero limit as the temperature goes to 0: the skyrmion probability is nonzero and constant at arbitrarily low temperatures and zero temperature. Hence there are skyrmion excitations at criticality at arbitrarily low energies and temperatures, including zero at zero temperature. Therefore skyrmion excitations contribute to quantum critical physics.

We have seen that skyrmions are relevant at criticality as the critical point is associated with skyrmion gap collapse and they have a nonzero probability to be excited at arbitrarily low temperature at criticality. On the other hand, skyrmions have nonzero conserved topological number while the ground state has zero skyrmion number. Absent any external sources that can couple directly to skyrmion number, they will always be created in equal numbers of skyrmions and antiskyrmions. Therefore, in order to study the effect of skyrmions and antiskyrmions we need to include configurations with equal number of skyrmions and antiskyrmions in the partition function or path integral. We found a time independent solution to the equations of motion given by

$$w_t^{(n)} = e^{i\varphi} \tan \left[\left(\frac{\lambda}{z - a} \right)^n + \left(\frac{\lambda^*}{z^* - a^*} \right)^n + \frac{\theta}{2} \right]$$
 (11)

where λ is the size of the configuration, θ and φ are the arbitrary directions of the configurations, a is the arbitrary position of the configuration and n is an integer. This configuration is topologically trivial because it has q = 0 as obtained from (4). On the other hand, it is composed of arbitrary superpositions of equal numbers of skyrmions and antiskyrmions with $q = \pm n$, i.e. the precise superpositions we need to sum over in the path integral for the q=0 sector. Since this configurations is made of topologically nontrivial skyrmions and antiskyrmions, we dub it a topolon. While the argument of the tangent is obviously a sum of an n skyrmion and an nantiskyrmion, it appears to not be a fully general one as all the skyrmions are at the same position. By starting with a fully general skyrmion configuration and making a change of variables to an effective "center of mass" coordinate, it follows that the results are the same as having all skyrmions at the same place.

The topolon with spatial and temporal size λ has Euclidean action (6)

$$S_E^t = \int_0^{\lambda} d\tau \frac{8\pi}{\lambda g_{1/\lambda}} \left(\lambda \Lambda\right)^{2n} \simeq \frac{8\pi\lambda\Lambda}{g_{\Lambda}} \left(\lambda \Lambda\right)^{2n} + \mathcal{O}(g_{\Lambda}^0) \tag{12}$$

The partition function including topolon configurations is given by $\mathcal{Z}=\sum_{n=0}^{\infty}\mathcal{Z}_n$ where

$$\mathcal{Z}_0 = \int \frac{\mathcal{D}\nu \mathcal{D}\nu^*}{(1+|\nu|^2)^2} e^{-S_E[\nu]}$$
 (13)

is the usual partition function for the nonlinear sigma model with no topolons and only the spin wave like fields ν and S_E is the Euclidean action for the nonlinear sigma model in terms of the stereographic projection variables (6). We also have that

$$\mathcal{Z}_{n\neq 0} = \int \frac{\mathcal{D}\nu \mathcal{D}\nu^*}{(1+|w_t^{(n)}+\nu|^2)^2} \frac{d^2a}{A} \frac{d\Omega}{4\pi} \frac{d\lambda}{1/\Lambda} e^{-S_E[w_t^{(n)}+\nu]}.$$

The $Z_{n\neq 0}$ is the path integral with the n topolons with spin waves ν . Besides integrating over the spin wave configurations, we must integrate over the topolon parameters: its size λ normalized to the lattice spacing $1/\Lambda$, its position a normalized to the area A of the system, and over the solid angle of its orientation normalized to 4π .

In order to renormalize the nonlinear sigma model, we integrate the spin wave degrees of freedom ν with momenta between the microscopic cutoff Λ and a lower cutoff or renormalization scale $\mu[6]$. We also integrate topolons of size between the microscopic minimum length $1/\Lambda$ and a new larger renormalization length $1/\mu$. We thus obtain a double expansion in $(1-\mu/\Lambda)$ and the coupling constant which leads to the renormalized action, the renormalized spin stiffness and the beta function

$$\begin{split} S_{\mathrm{ren}} &= \frac{2\mu}{g_{\mu}} \int d^3x \frac{\partial_{\mu}\nu\partial_{\mu}\nu^*}{(1+|\nu|^2)^2} \simeq \frac{2\Lambda}{g_{\Lambda}} \int d^3x \partial_{\mu}\nu\partial_{\mu}\nu^* \times \\ &\left\{ 1 - \left(1 - \frac{\mu}{\Lambda}\right) \frac{g_{\Lambda}}{2\pi^2} + \left(1 - \frac{\mu}{\Lambda}\right) \frac{1}{3(e^{8\pi/g_{\Lambda}} - 1)} \right\} \\ &\rho_s(\mu) &= \frac{\mu}{g_{\mu}} = \frac{\Lambda}{g_{\Lambda}} \times \\ &\left\{ 1 - \left(1 - \frac{\mu}{\Lambda}\right) \frac{g_{\Lambda}}{2\pi^2} + \left(1 - \frac{\mu}{\Lambda}\right) \frac{1}{3(e^{8\pi/g_{\Lambda}} - 1)} \right\} \\ &\beta(g) &= \mu \frac{\partial g}{\partial \mu} \bigg|_{\Lambda = \mu} = g - \frac{g^2}{2\pi^2} + \frac{g}{3(e^{8\pi/g} - 1)} \,. \end{split}$$

The last term in the spin stiffness and in the beta function is the contribution from the topolons and the rest is the contribution of the spin waves. The coupling constant at the quantum critical point $g_c \simeq 23.0764$ is obtained from $\beta(q_c) = 0$.

The correlation length at scale μ is given by [6]

$$\xi \sim \mu^{-1} \exp \left[\int_{g_c}^{g_{\mu}} \frac{dg}{\beta(g)} \right] \sim \mu^{-1} \left(g_c - g_{\mu} \right)^{1/\beta'(g_c)} .$$
 (14)

The correlation length exponent is $\nu = -1/\beta'(g_c) \equiv -(d\beta/dg|_{g=g_c})^{-1}$. The correlation length exponent with topolon contributions evaluates to $\nu = 0.9297$. The $d = 2 + \epsilon$ expansion of the O(N) vector model, which agrees with the 1/N expansion for large N, gives $\nu = 0.5[16]$.

We note that our value is larger than the accepted numerical evaluations of critical exponents in the Heisenberg model, $\nu=0.71125[15]$, but about as close to this accepted Heisenberg value than the $2+\epsilon$ expansion or the 1/N expansion. We conjecture that the difference between our value and the Heisenberg value is real and attributable to quantum critical degrees of freedom.

Goldstone renormalizations of the ordering direction $\sigma=n_3$, and hence of the anomalous dimension η , are notoriously inaccurate. The one loop approximation leads to a value of $\eta=2$, thousands of percent different from the accepted numerical value of $\eta\simeq 0.0375[15]$. The large N approximation, which sums bubble diagrams, is a lot more accurate. To order 1/N one obtains $\eta=8/(3\pi^2N)\simeq 0.09$ for N=3. We now calculate the value of η from topological nontrivial configurations

$$\begin{split} \langle n_3^2 \rangle &= Z = 1 - \langle n_1^2 + n_2^2 \rangle = 1 - \left\langle \frac{4|w|^2}{(1+|w|^2)^2} \right\rangle \\ &\simeq 1 - \frac{2}{3} \frac{1 - \mu/\Lambda}{e^{8\pi/g_\Lambda} - 1} \Rightarrow \eta(g) = \frac{\mu}{Z} \frac{\partial Z}{\partial \mu} \Big|_{\Lambda = \mu} \simeq \frac{2}{3(e^{8\pi/g} - 1)} \end{split}$$

For the anomalous dimension at the quantum critical point we obtain $\eta(g_c)=0.3381$. On the other hand, we have seen that spin wave contributions tend to give quite large and nonsensical values of η . In fact so large as to wash out the momentum dependence of the propagator. Hence, to calculate η , spin wave contributions prove to be tough to control. Our calculation gives a value quite larger than the accepted numerical value. We have recently calculated [17] the unique value of η that follows from quantum critical fractionalization into spinons and find $\eta=1$. While our value obtained from topolons is far from 1, it is a lot closer than the accepted numerical Heisenberg value and the 1/N value.

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